Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.86

Global applicability domain: Inside

Local applicability domain index: 4.73e-01

Confidence level: 6.03e-01

Nearest Neighbors from the Training Set

Image not found
Chloropicrin
Measured: 2.09
Predicted: 1.86

Image not found
Trichloroacetic acid
Measured: 1.33
Predicted: 1.41

Image not found
2,2,2-Trichloroacetamide
Measured: 1.04
Predicted: 1.12

Image not found
Dichloromethane
Measured: 1.25
Predicted: 1.43

Image not found
4-Methylthiazole
Measured: 0.97
Predicted: 1.78